Submitted to *Macromolecules*

Version of March 17, 2004

Supporting Information

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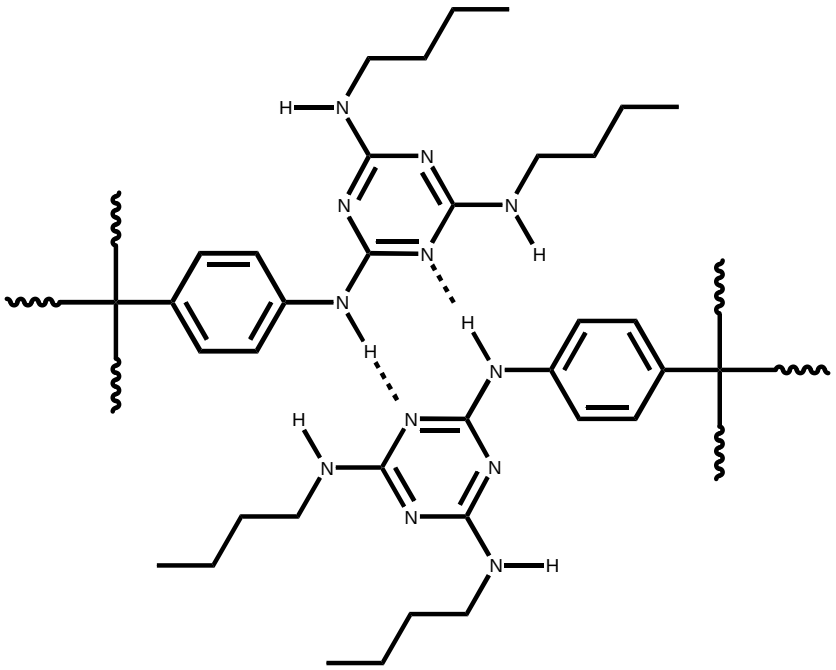
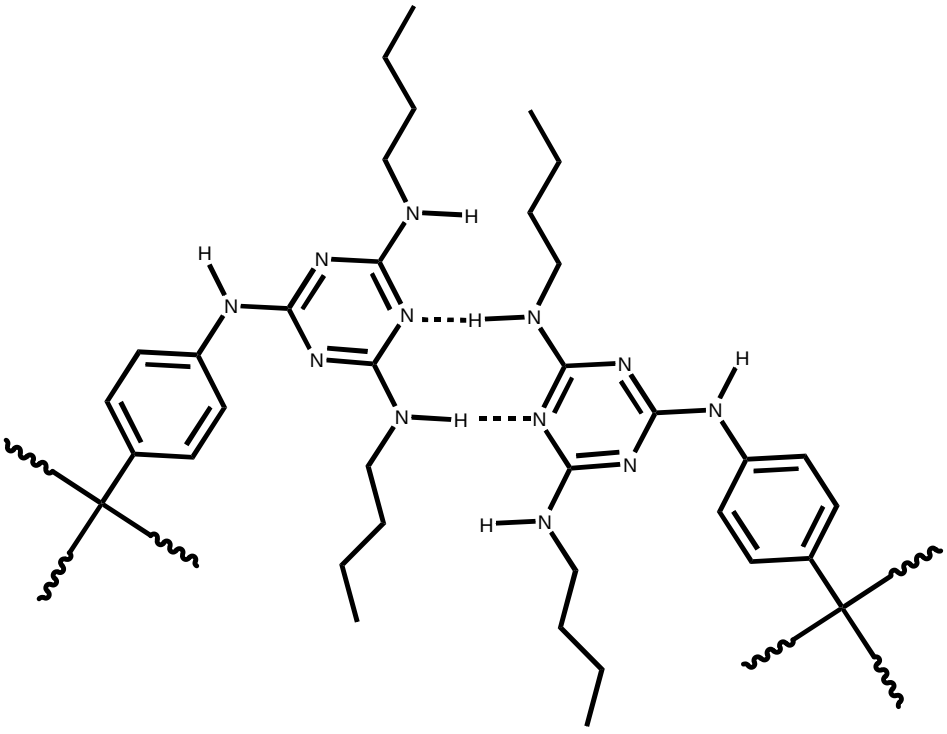
Tetrakis[4-[[4,6-bis(butylamino)-1,3,5-triazin-2-yl]amino]phenyl]methane crystallizes as an inclusion compounds with 10 dioxane molecules in the tetragonal space group I-4 with $a = b = 11.8715(30$ Å, $c = 40.004(2)$ Å and $V = 5637.9(4)$ Å^3. Each molecule participates in a total of 16 hydrogen bonds with eight neighbors (figure **7**) according two different motifs of association (figure **1**). Motif **1** engages two amino functions between the two phenyl rings while motif **2** involves two amino functions from the butylamine chains. Figure **2** shows the hydrogen bonding recognition for one arm of the molecule. Pairs of hydrogen bonds link a central tecton (in red) with tecton in blue according to motif **1** and with tecton in green according to motif **2**. The green and blue tectons are also hydrogen-bonded via the motif **1**. Together, a central tecton and its four hydrogen-bonded neighbors linked via motif **1** (figure **3**) define a simple square planar network lying in parallel to the (*a*, *b*) crystallographic plane (figure **4**). A same network in the same plane but tilted at 45 degrees (figure **6**) is defined by a central tecton and its four hydrogen-bonded networks via motif **2** (figure **5**). The resulting topology is the superposition of the two square-planar networks giving planar networks running in parallel to the to the (*a*, *b*) crystallographic plane (figure **8**). The hydrogen-bonded molecules are stacked in layers with only van der Waals interactions between the layers via the butylamine moieties (figure **9**).

The resulting structure is anisotropic in the interactions with the hydrogen bonds restrained in the layers while weaker van der Waals contacts assure the cohesion between the layers. The butylamine chains are not confined between the sheets but lye also within them (figure **11**). Approximately 47 % of the volume in the lattice remains available for including the dioxane guest molecules in interconnected channels. These channels are positioned in planes perpendicular to the *c*-axis while no porosity is observed along the *c* axis. Figure **10** shows that these channels have a cross sections of approximately 5×12 Å at the narrowest points.

X-ray diffraction powder diagrams for tecton **6**, **7**, **8**, **9** and **10** were measured between 2 and 60 degrees in 2θ (figure 12) using CoKα radiation (λ = 1.790 Å). Each diagram displays a braod peak in the range 20 – 30 degrees in 2θ that is characteristic of amorphous system and a narrowest peak at low angle (figure **13**) with a position varying with the alkyl chain length as plotted in figure **14**.



Motif **1**



Motif **2**

Figure **1:** View of the two different motifs of hydrogen bond observed in the structure of tetrakis[4-[[4,6-bis(butylamino)-1,3,5-triazin-2-yl]amino]phenyl]methane. Motif **1** engages two amino functions between the two phenyl rings while motif **2** involves two amino functions from the butylamine moitie.

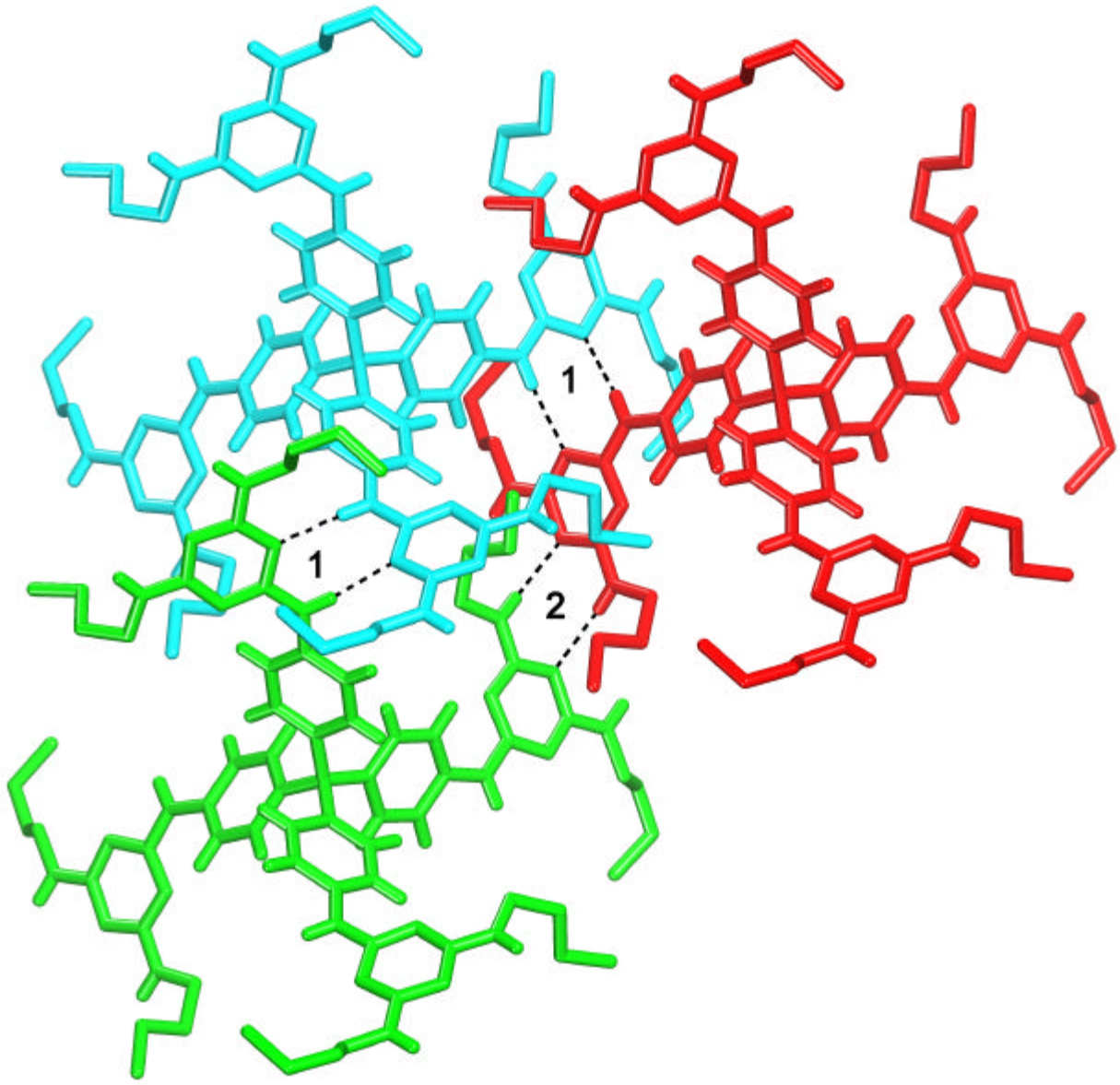


Figure **2:** View of the structure of tetrakis[4-[[4,6-bis(butylamino)-1,3,5-triazin-2-yl]amino]phenyl]methane showing the hydrogen bonding recognition for one arm of the molecule. Pairs of hydrogen bonds link the central tecton in red with the tecton in blue according to motif **1** and with the tecton in green according to motif **2**. The green and blue tectons are also hydrogen-bonded via the motif **1**. Each arm of the tecton is involved in 4 hydrogen bonds, giving a total of 16 hydrogen bonds for the whole four-armed molecule. Hydrogen bonds appear as broken lines. Hydrogen atoms of the tetraphenylmethane core and the butyl chains have been omitted for clarity.

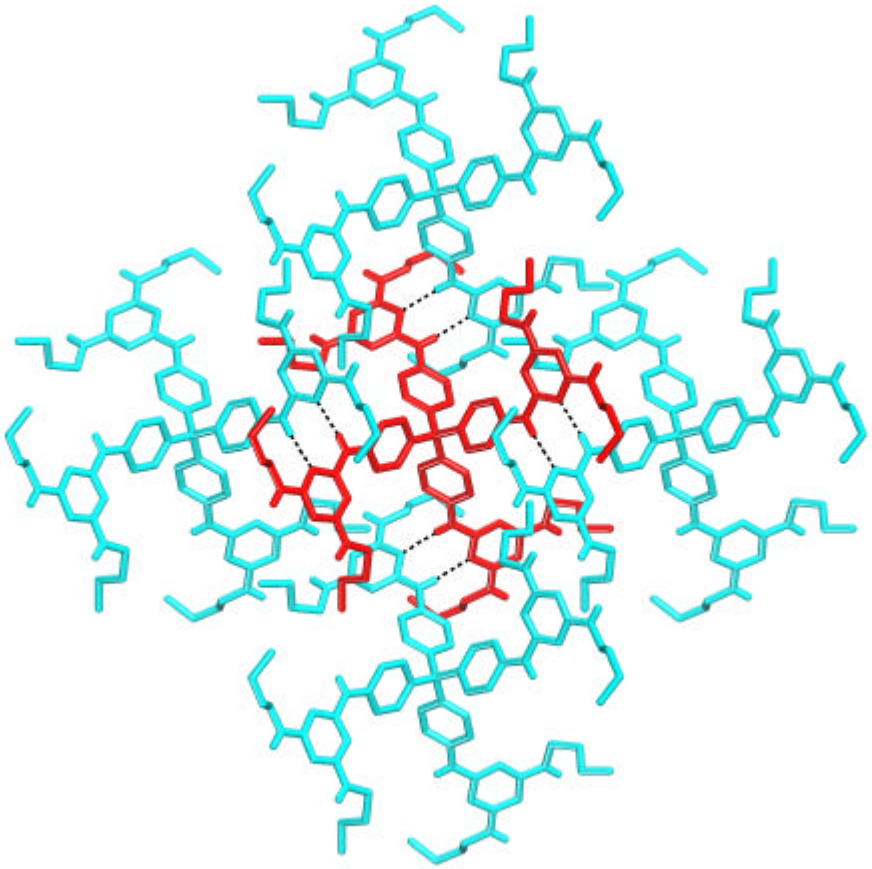


Figure **3:** View of the structure of tetrakis[4-[[4,6-bis(butylamino)-1,3,5-triazin-2-yl]amino]phenyl]methane along the *c* axis showing the hydrogen bonding recognition of a central molecule in red linked by pair of hydrogen bonds according to the motif **1** with four neighbors molecules in cyan. Hydrogen bonds appear as broken lines. Hydrogen atoms of the tetraphenylmethane core and the butyl chains have been omitted for clarity.

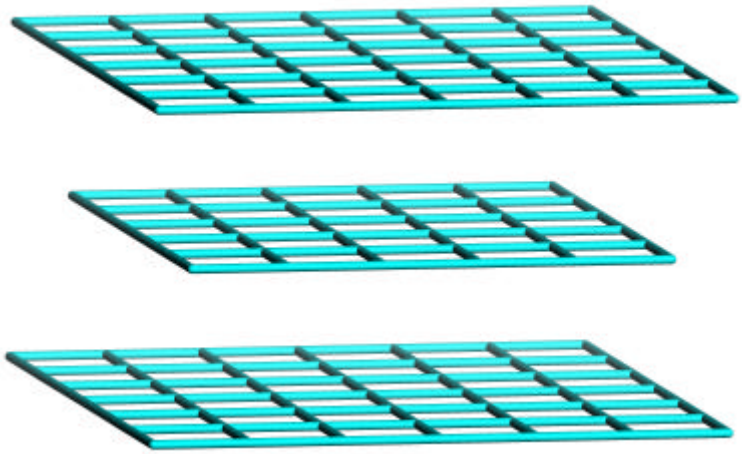


Figure **4:** Representation of the square network generated by association of tetrakis[4-[[4,6-bis(butylamino)-1,3,5-triazin-2-yl]amino]phenyl]methane according to the motif **1**. In this drawing, the central carbon atom of each tetraphenylmethane moieties lies at the intersection of solid lines that represent hydrogen bonding to four neighbors.

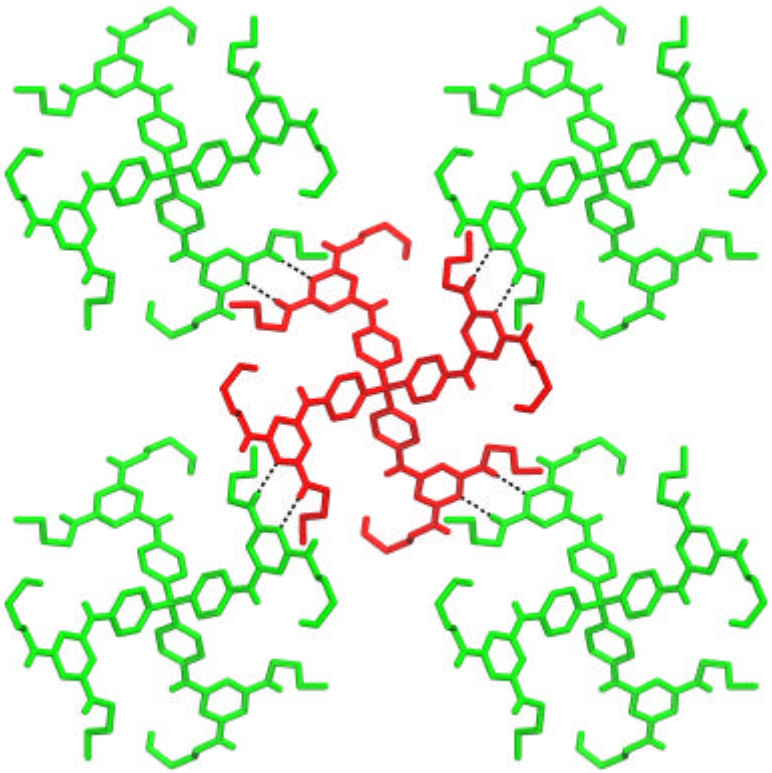


Figure **5:** View of the structure of tetrakis[4-[[4,6-bis(butylamino)-1,3,5-triazin-2-yl]amino]phenyl]methane along the *c* axis showing the hydrogen bonding recognition of a central molecule in red linked by pair of hydrogen bonds according to the motif **2** with four neighbors molecules in green. Hydrogen bonds appear as broken lines. Hydrogen atoms of the tetraphenylmethane core and the butyl chains have been omitted for clarity.

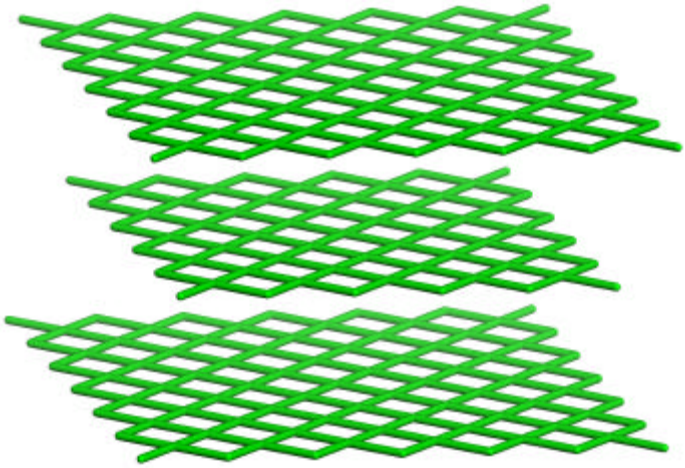


Figure **6:** Representation of the square network generated by association of tetrakis[4-[[4,6-bis(butylamino)-1,3,5-triazin-2-yl]amino]phenyl]methane according to the motif **2**. In this drawing, the central carbon atom of each tetraphenylmethane moieties lies at the intersection of solid lines that represent hydrogen bonding to four neighbors.

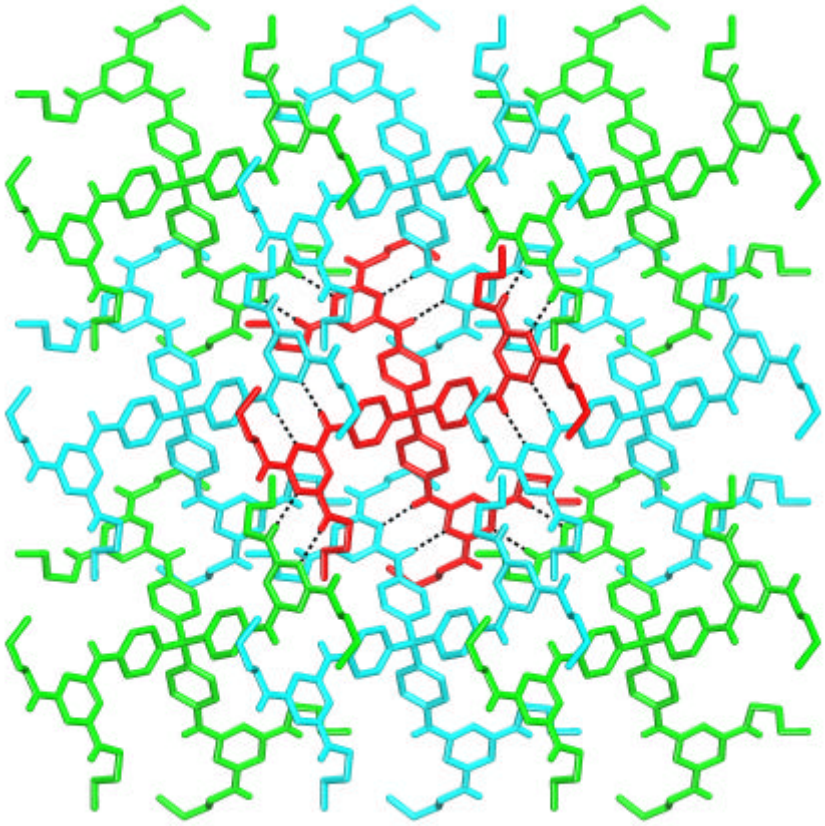


Figure **7:** View of the structure of tetrakis[4-[[4,6-bis(butylamino)-1,3,5-triazin-2-yl]amino]phenyl]methane along the *c* axis showing the recognition involving 16 hydrogen bonds. Pairs of hydrogen bonds link the central tecton in red with the tecton in blue according to motif **1** and with the tecton in green according to motif **2**. Hydrogen bonds appear as broken lines. Hydrogen atoms of the tetraphenylmethane core and the butyl chains have been omitted for clarity.

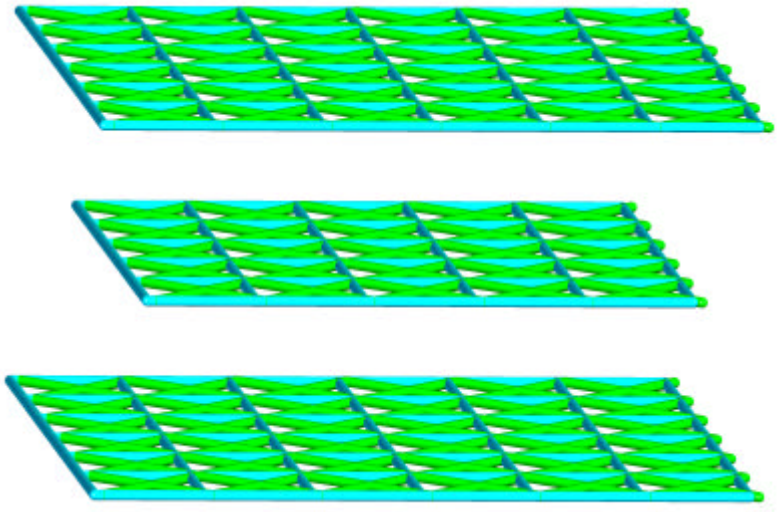


Figure **8:** Representation of the square network generated by association of tetrakis[4-[[4,6-bis(butylamino)-1,3,5-triazin-2-yl]amino]phenyl]methane according to the motifs **1** and **2**. In this drawing, the central carbon atom of each tetraphenylmethane moieties lies at the intersection of solid lines that represent hydrogen bonding to eight neighbors.

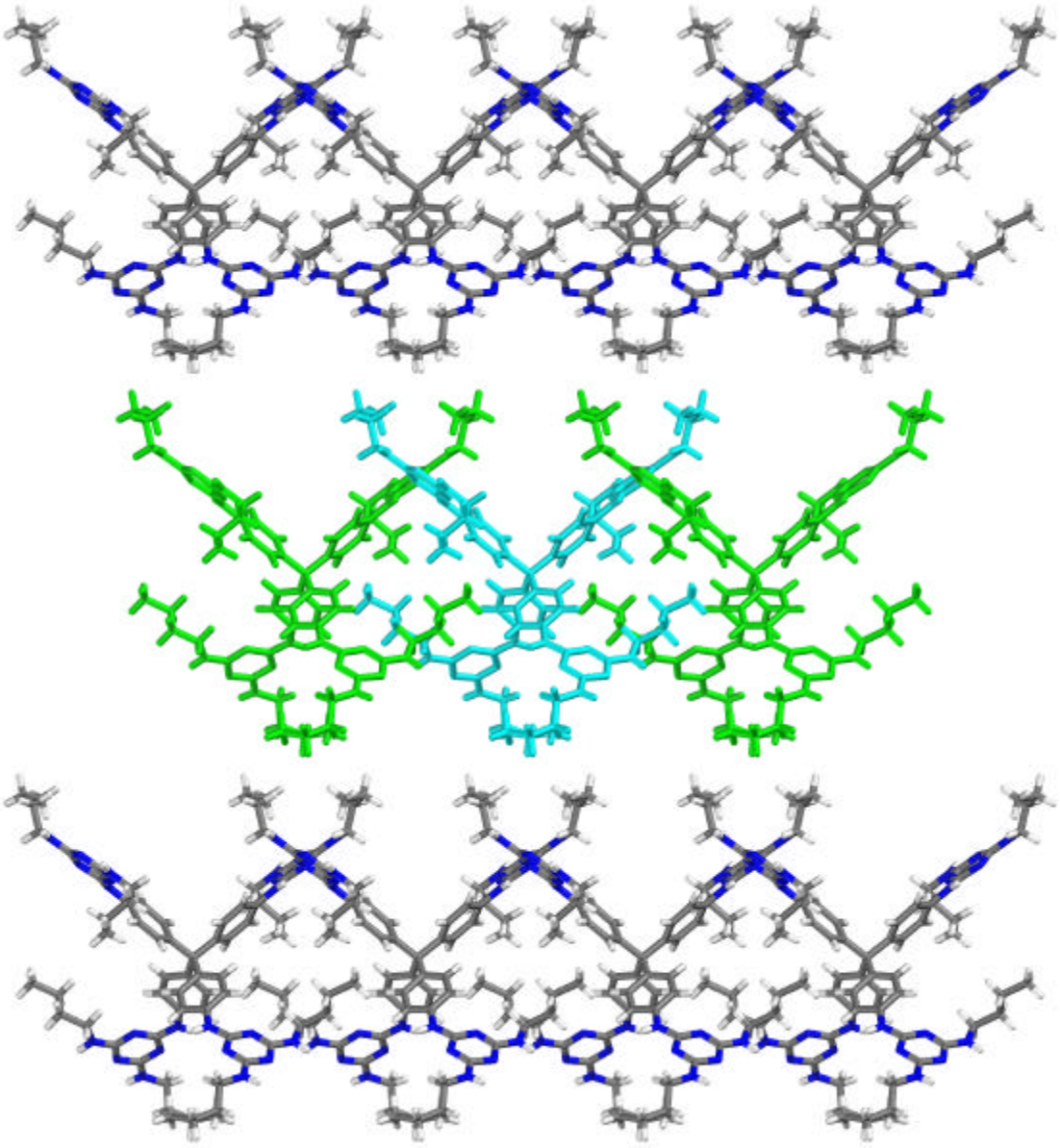


Figure **9:** View of the structure of tetrakis[4-[[4,6-bis(butylamino)-1,3,5-triazin-2-yl]amino]phenyl]methane along the *b* axis showing three different layers of hydrogen bonded molecules. The layer are only linked via van der Waals interactions between the butylamine moieties.

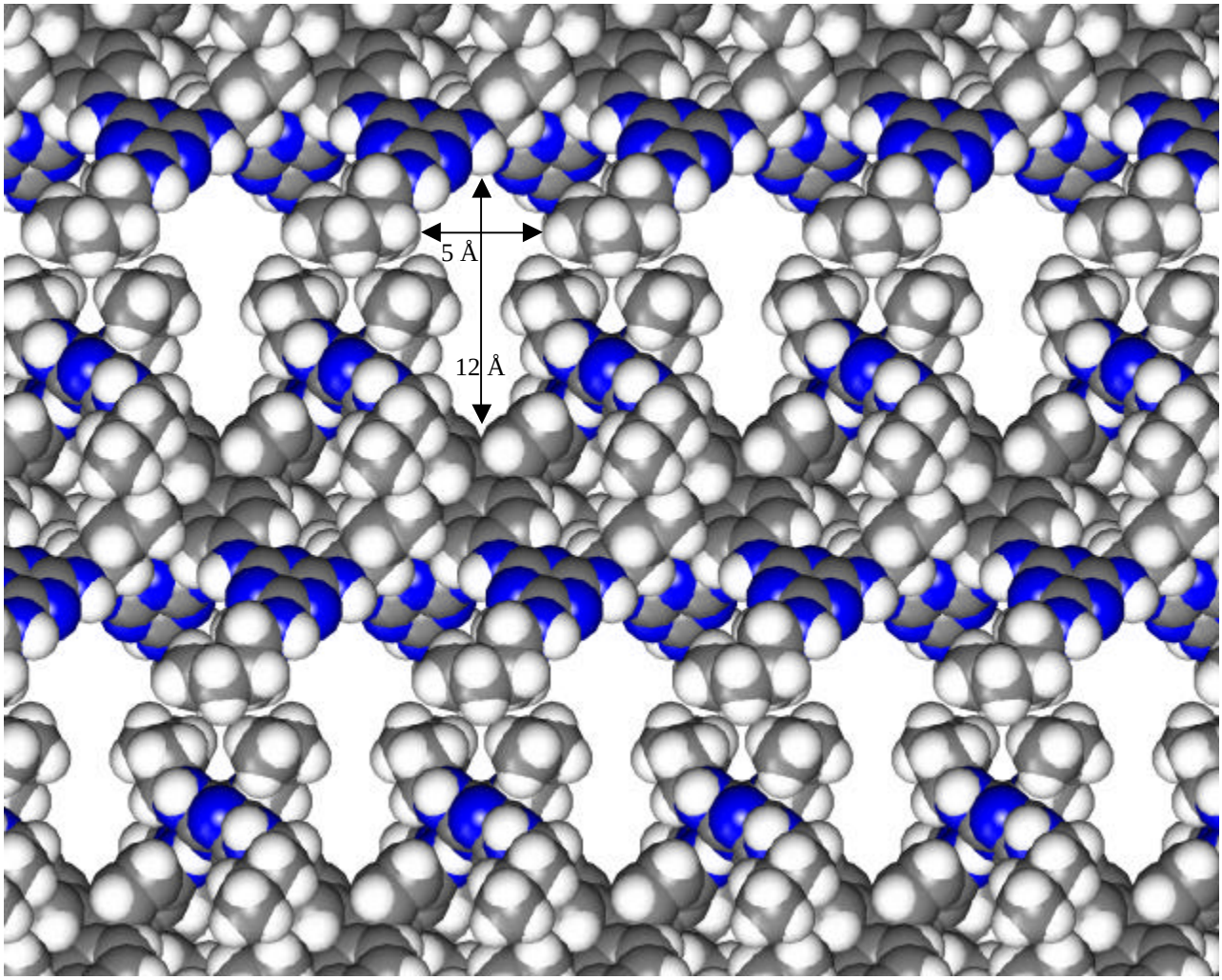


Figure **10:** View of the structure of tetrakis[4-[[4,6-bis(butylamino)-1,3,5-triazin-2-yl]amino]phenyl]methane along the *b* axis showing a 4 × 2 × 1 array of unit cells. Dioxane guest molecules have been omitted and atoms are shown as sphere of van der Waals radii in order to reveal the cross sections of the channels. Atoms of hydrogen appear in white, atoms of carbon in light gray and atoms of nitrogen in blue.

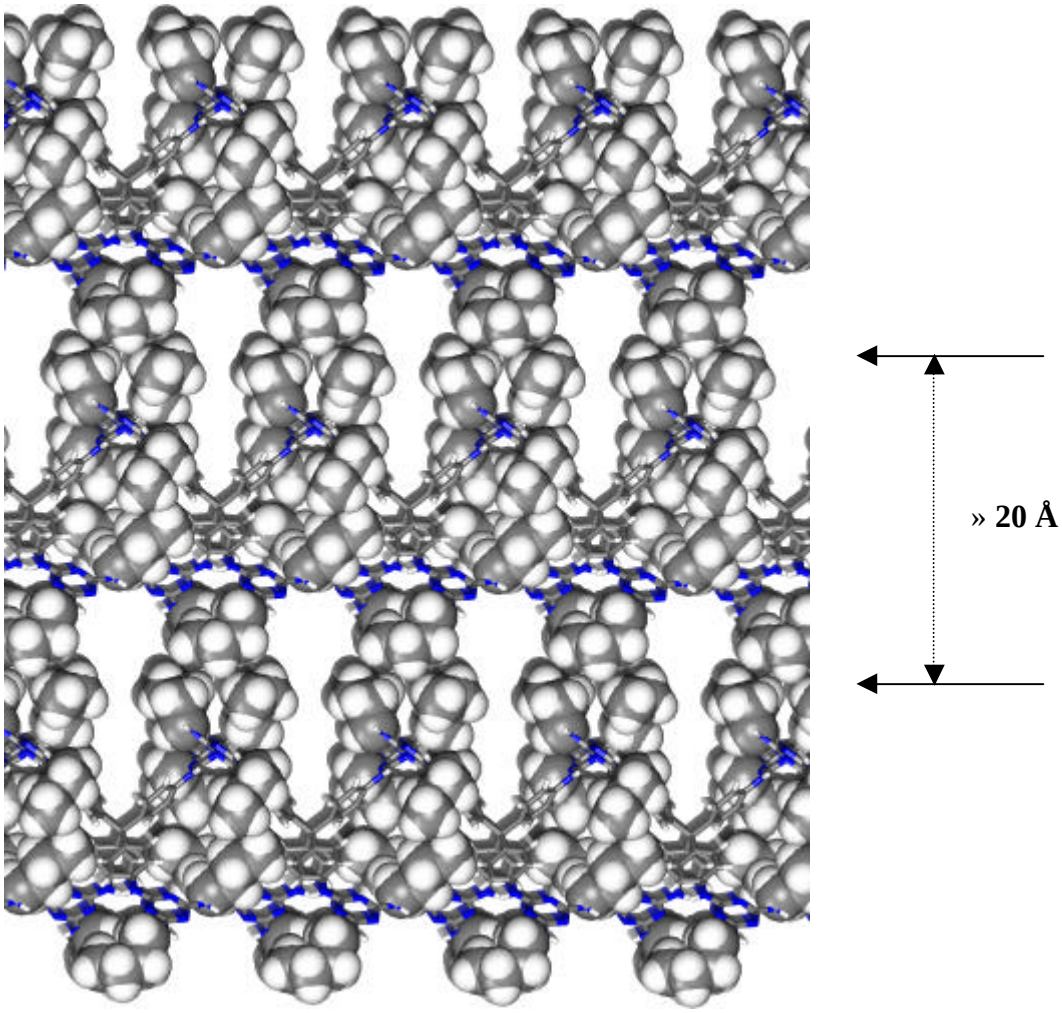


Figure **11**: View of the structure of tetrakis[4-[[4,6-bis(butylamino)-1,3,5-triazin-2-yl]amino]phenyl]methane along the *b* axis showing a 4 × 2 × 2 array of unit cells. Dioxane guest molecules have been omitted and atoms of the butylamine moieties are shown as sphere of van der Waals radii to show the location of the aliphatic chains in the structure. Atoms of hydrogen appear in white, atoms of carbon in light gray and atoms of nitrogen in blue.

Université de Montréal

CRYSTAL AND MOLECULAR STRUCTURE OF

C109 H180 N24 O20 COMPOUND (JIW300)

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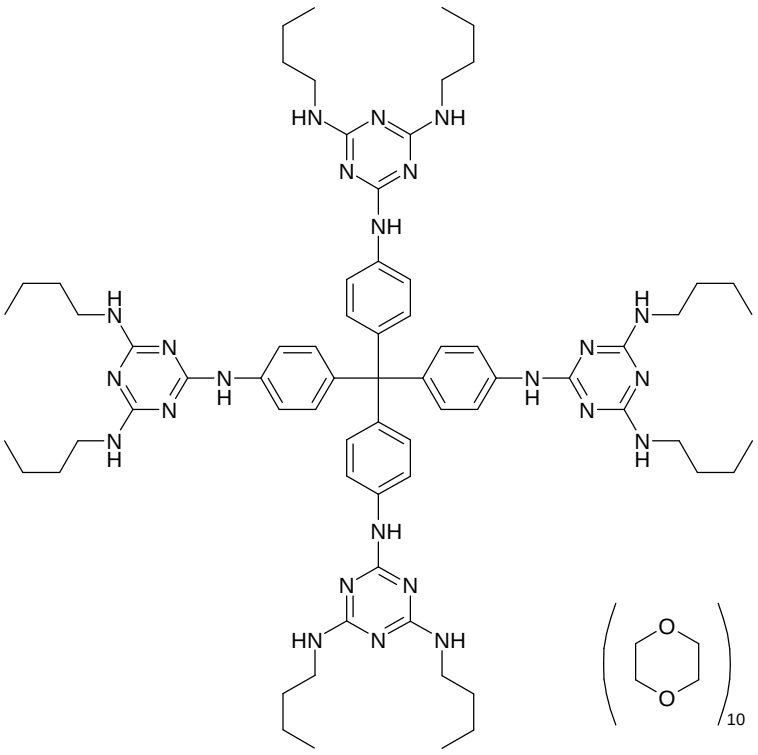


Structure solved and refined in the laboratory of X-ray diffraction Université de Montréal by Dr. Thierry Maris.

Table 1. Crystal data and structure refinement for C109 H180 N24 O20.

Identification code	JIW300
Empirical formula	C109 H180 N24 O20
Formula weight	2146.77
Temperature	226(2)K
Wavelength	1.54178 Å
Crystal system	Tetragonal
Space group	I-4
Unit cell dimensions	a = 11.8715(3) Å $\alpha = 90^\circ$ b = 11.8715(3) Å $\beta = 90^\circ$ c = 40.004(2) Å $\gamma = 90^\circ$
Volume	5637.9(4)Å^3
Z	2
Density (calculated)	1.265 Mg/m^3
Absorption coefficient	0.715 mm^{-1}
F(000)	2324
Crystal size	0.55 x 0.40 x 0.40 mm
Theta range for data collection	2.21 to 58.88°
Index ranges	$-13 \leq h \leq 12$, $-12 \leq k \leq 13$, $-44 \leq \ell \leq 40$
Reflections collected	36656
Independent reflections	4045 [R_{int} = 0.076]
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.8600 and 0.2100
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4045 / 450 / 403
Goodness-of-fit on F^2	1.077
Final R indices [I>2sigma(I)]	R_1 = 0.0868, wR_2 = 0.2183
R indices (all data)	R_1 = 0.0876, wR_2 = 0.2195
Largest diff. Peak and hole	0.467 and –0.317 e/Å^3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for C109 H180 N24 O20.

U_{eq} is defined as one third of the trace of the orthogonalized Uij tensor.

	Occ.	X	y	z	U_{eq}
C(1)	1	0	10000	0	40(2)
N(1)	1	3687(4)	9333(3)	922(1)	44(1)
C(2)	1	995(5)	9760(4)	242(1)	45(1)
N(2)	1	5110(4)	8555(4)	1226(1)	45(1)
C(3)	1	1354(5)	10602(5)	461(1)	47(1)
N(3)	1	3624(5)	7396(4)	1013(1)	55(1)
C(4)	1	2216(5)	10454(4)	684(1)	42(1)
N(4)	1	5044(5)	6583(5)	1362(1)	59(1)
C(5)	1	2771(4)	9424(5)	696(1)	43(1)
N(5)	1	3693(6)	5497(5)	1123(2)	75(2)
C(6)	1	2437(5)	8576(5)	484(2)	51(1)
N(6)	1	6431(6)	7739(4)	1567(1)	67(2)
C(7)	1	1570(5)	8772(5)	255(2)	51(1)
C(9)	1	4129(5)	8375(5)	1055(1)	44(1)
C(10)	1	5509(5)	7631(4)	1370(2)	47(1)
C(11)	1	4134(5)	6535(5)	1168(2)	51(1)
C(12)	1	6943(6)	8820(5)	1661(2)	64(2)
C(13)	1	7006(11)	8979(9)	2029(2)	103(3)
C(14)	1	7512(11)	10012(10)	2145(3)	107(3)
C(15)	1	6729(12)	11041(12)	2054(4)	135(5)
C(16)	1	2735(7)	5234(5)	910(2)	76(2)
C(17A)	0.39(3)	3140(20)	5020(30)	571(5)	98(10)
C(17)	0.61(3)	2815(18)	4011(14)	757(6)	120(9)
C(18)	1	3749(15)	3985(12)	515(3)	162(7)
C(19)	1	3792(15)	2809(12)	341(3)	284(18)
O(50A)	0.692(11)	10922(9)	7388(16)	3026(4)	155(5)
C(50A)	0.692(11)	9834(10)	7229(16)	3137(3)	126(4)
C(51A)	0.692(11)	9072(14)	8135(17)	3008(3)	144(5)
O(51A)	0.692(11)	9041(12)	7982(18)	2667(3)	171(5)
C(52A)	0.692(11)	10051(14)	8441(18)	2564(3)	158(4)
C(53A)	0.692(11)	10786(14)	7500(20)	2685(3)	161(4)
O(50B)	0.308(11)	11090(30)	7880(30)	2941(8)	155(5)
C(50B)	0.308(11)	10340(30)	8760(30)	2918(7)	126(4)
C(51B)	0.308(11)	9210(20)	8230(40)	2858(9)	144(5)
O(51B)	0.308(11)	9290(30)	7850(40)	2532(7)	171(5)
C(52B)	0.308(11)	9830(30)	6830(40)	2570(8)	158(4)
C(53B)	0.308(11)	10960(30)	7350(40)	2637(11)	161(4)
O(60A)	0.500(8)	285(14)	8493(12)	1140(4)	107(3)
C(60A)	0.500(8)	1027(13)	8502(12)	1404(3)	79(2)
C(61A)	0.500(8)	845(15)	7707(16)	1687(3)	103(4)
O(61A)	0.500(8)	-242(14)	7316(19)	1702(3)	151(5)
C(62A)	0.500(8)	-420(20)	6900(20)	1384(4)	130(4)
C(63A)	0.500(8)	130(20)	7364(14)	1077(3)	120(4)
O(60B)	0.500(8)	617(12)	8194(13)	1179(3)	107(3)
C(60B)	0.500(8)	20(14)	8607(10)	1451(3)	79(2)
C(61B)	0.500(8)	90(20)	7654(12)	1696(3)	103(4)
O(61B)	0.500(8)	-587(16)	6786(16)	1580(4)	151(5)
C(62B)	0.500(8)	-110(20)	6529(14)	1276(4)	130(4)
C(63B)	0.500(8)	-170(20)	7489(15)	1032(4)	120(4)
C(70A)	0.783(18)	9373(17)	4238(18)	347(4)	184(8)
C(71A)	0.783(18)	10205(15)	4018(8)	65(4)	142(5)
C(70B)	0.217(18)	9030(30)	5050(60)	342(13)	184(8)
C(71B)	0.217(18)	9300(40)	4250(30)	55(11)	142(5)
O(70)	1	10000	5000	560(3)	143(4)
O(71)	1	10000	5000	-141(3)	251(11)

Table 3. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for C109 H180 N24 O20.

	Occ.	X	y	z	U_{eq}
H(1A)	1	4002	9963	983	52
H(3)	1	988	11303	454	56
H(4)	1	2430	11043	828	50
H(5A)	1	4009	4941	1229	90
H(6)	1	2789	7867	493	61
H(6A)	1	6741	7126	1644	80
H(7)	1	1377	8196	105	61
H(12A)	1	6501	9434	1564	77
H(12B)	1	7705	8860	1567	77
H(13A)	1	6240	8938	2119	124
H(13B)	1	7431	8348	2124	124
H(14A)	1	8252	10111	2040	129
H(14B)	1	7619	9978	2388	129
H(15A)	1	6542	11013	1818	202
H(15B)	1	7121	11739	2102	202
H(15C)	1	6044	11002	2185	202
H(16A)	1	2695	5785	728	91
H(16B)	1	2040	5297	1041	91
H(17A)	0.39(3)	2492	5026	420	117
H(17B)	0.39(3)	3633	5644	506	117
H(17A)	0.61(3)	2950	3461	936	144
H(17B)	0.61(3)	2106	3817	646	144
H(18A)	1	4463	4128	630	194
H(18B)	1	3641	4576	347	194
H(19A)	1	4001	2239	503	426
H(19B)	1	4344	2825	162	426
H(19C)	1	3057	2632	249	426
H(50A)	0.692(11)	9822	7232	3382	152
H(50B)	0.692(11)	9561	6493	3060	152
H(51A)	0.692(11)	8316	8061	3104	173
H(51B)	0.692(11)	9370	8882	3063	173
H(52A)	0.692(11)	10218	9155	2676	189
H(52B)	0.692(11)	10089	8539	2321	189
H(53A)	0.692(11)	10475	6788	2600	193
H(53B)	0.692(11)	11534	7590	2585	193
H(50A)	0.308(11)	10536	9265	2732	152
H(50B)	0.308(11)	10330	9202	3126	152
H(51C)	0.308(11)	)9082	7599	3013	173
H(51D)	0.308(11)	)8599	8777	2883	173
H(52C)	0.308(11)	)9817	6375	2366	189
H(52D)	0.308(11)	)9541	6395	2759	189
H(53C)	0.308(11)	11528	6754	2621	193
H(53D)	0.308(11)	11116	7895	2460	193
H(60A)	0.500(8)	1034	9266	1496	94
H(60B)	0.500(8)	1781	8357	1314	94
H(61A)	0.500(8)	1360	7067	1664	124
H(61B)	0.500(8)	1026	8091	1898	124
H(62A)	0.500(8)	-1236	6948	1345	156
H(62B)	0.500(8)	-235	6099	1392	156
H(63A)	0.500(8)	857	6992	1038	144
H(63B)	0.500(8)	-348	7255	881	144
H(60C)	0.500(8)	-763	8771	1390	94
H(60D)	0.500(8)	371	9291	1540	94
H(61C)	0.500(8)	870	7396	1716	124
H(61D)	0.500(8)	-169	7904	1916	124
H(62C)	0.500(8)	-494	5875	1181	156
H(62D)	0.500(8)	683	6323	1311	156
H(63C)	0.500(8)	59	7260	807	144
H(63D)	0.500(8)	-919	7830	1025	144

H(70A)	0.783(18)	8682	4590	263	221
H(70B)	0.783(18)	9180	3540	465	221
H(71A)	0.783(18)	10983	3994	146	170
H(71B)	0.783(18)	10032	3318	-54	170
H(70C)	0.217(18)	8911	5818	258	221
H(70D)	0.217(18)	8345	4808	460	221
H(71C)	0.217(18)	9719	3582	132	170
H(71D)	0.217(18)	8626	4008	-66	170

Table 4. Anisotropic parameters ($Å^2$ x 10^3) for C109 H180 N24 O20.
The anisotropic displacement factor exponent takes the form:

$$-2\pi^2 [h^2 a^{*2} U_{11} + \ldots + 2 h k a^* b^* U_{12}]$$

	U11	U22	U33	U23	U13	U12
C(1)	35(3)	35(3)	50(5)	0	0	0
N(1)	44(2)	26(2)	61(2)	2(2)	-7(2)	3(2)
C(2)	45(3)	42(3)	47(3)	0(2)	19(2)	0(2)
N(2)	48(2)	36(2)	51(2)	2(2)	-3(2)	7(2)
C(3)	50(3)	34(3)	55(3)	1(2)	-9(3)	-1(2)
N(3)	65(3)	36(3)	65(3)	-4(2)	-15(3)	3(2)
C(4)	51(3)	28(3)	46(3)	4(2)	2(2)	-4(2)
N(4)	70(3)	52(3)	55(2)	-1(2)	-7(3)	6(2)
C(5)	30(3)	48(3)	51(3)	1(2)	3(2)	3(2)
N(5)	76(4)	39(3)	109(5)	5(3)	-17(3)	-1(3)
C(6)	48(3)	42(3)	64(3)	-4(3)	-6(3)	8(2)
N(6)	92(4)	30(2)	78(3)	2(2)	-30(3)	14(3)
C(7)	50(3)	34(3)	68(3)	-12(2)	-9(3)	-6(2)
C(9)	42(3)	43(3)	47(3)	7(2)	0(2)	-6(2)
C(10)	52(3)	33(3)	55(3)	0(2)	-13(3)	8(2)
C(11)	60(3)	26(3)	66(3)	5(3)	-5(3)	-1(2)
C(12)	65(4)	47(3)	81(4)	8(3)	-34(3)	-8(3)
C(13)	128(8)	102(7)	80(5)	-17(5)	-29(6)	7(6)
C(14)	119(8)	107(7)	96(6)	-2(6)	-3(6)	-30(7)
C(15)	128(10)	128(10)	149(11)	13(8)	-44(9)	-5(8)
C(16)	82(5)	41(3)	106(5)	5(4)	-32(4)	-10(3)
C(17A)	84(15)	140(20)	65(12)	0(13)	0(10)	25(14)
C(17)	134(16)	72(10)	154(18)	35(11)	-58(14)	-58(10)
C(18)	198(18)	171(15)	115(9)	-35(10)	-44(12)	2(14)
C(19)	490(50)	179(19)	179(15)	-9(14)	-90(20)	-180(30)
O(50A)	82(6)	239(13)	145(9)	-46(9)	-30(6)	-53(7)
C(50A)	122(9)	188(11)	69(6)	-6(7)	2(6)	-56(6)
C(51A)	107(7)	221(12)	104(9)	-29(9)	-22(7)	-26(7)
O(51A)	119(7)	286(12)	107(8)	-28(8)	-22(7)	-4(7)
C(52A)	122(8)	252(12)	100(7)	-58(8)	-24(7)	-39(8)
C(53A)	90(7)	255(12)	137(8)	-65(9)	21(7)	-33(7)
O(50B)	82(6)	239(13)	145(9)	-46(9)	-30(6)	-53(7)
C(50B)	122(9)	188(11)	69(6)	-6(7)	2(6)	-56(6)
C(51B)	107(7)	221(12)	104(9)	-29(9)	-22(7)	-26(7)
O(51B)	119(7)	286(12)	107(8)	-28(8)	-22(7)	-4(7)
C(52B)	122(8)	252(12)	100(7)	-58(8)	-24(7)	-39(8)
C(53B)	90(7)	255(12)	137(8)	-65(9)	21(7)	-33(7)
O(60A)	123(8)	98(7)	99(4)	21(4)	1(4)	-32(6)
C(60A)	77(6)	72(5)	87(5)	5(4)	13(4)	-14(5)
C(61A)	127(10)	104(7)	79(5)	18(5)	-1(7)	-66(8)
O(61A)	175(10)	147(9)	133(7)	17(6)	10(7)	-106(8)
C(62A)	176(10)	115(9)	99(7)	27(6)	-32(6)	-87(8)
C(63A)	160(11)	111(6)	91(5)	39(5)	-60(7)	-68(7)
O(60B)	123(8)	98(7)	99(4)	21(4)	1(4)	-32(6)
C(60B)	77(6)	72(5)	87(5)	5(4)	13(4)	-14(5)
C(61B)	127(10)	104(7)	79(5)	18(5)	-1(7)	-66(8)
O(61B)	175(10)	147(9)	133(7)	17(6)	10(7)	-106(8)
C(62B)	176(10)	115(9)	99(7)	27(6)	-32(6)	-87(8)
C(63B)	160(11)	111(6)	91(5)	39(5)	-60(7)	-68(7)
C(70A)	266(15)	190(20)	100(6)	-31(8)	-71(8)	-83(13)
C(71A)	154(12)	60(6)	211(10)	-39(6)	-94(9)	23(7)
C(70B)	266(15)	190(20)	100(6)	-31(8)	-71(8)	-83(13)
C(71B)	154(12)	60(6)	211(10)	-39(6)	-94(9)	23(7)
O(70)	146(10)	157(11)	124(7)	0	0	-70(8)
O(71)	520(40)	97(8)	139(10)	0	0	3(13)

Table 5. Bond lengths [Å] and angles [°] for C109 H180 N24 O20

C(1)-C(2)#1	1.554(6)	C(70a)-O(70)	1.450(4)
C(1)-C(2)	1.554(6)	C(70a)-C(71a)	1.521(5)
C(1)-C(2)#2	1.554(6)	C(71a)-O(71)	1.449(4)
C(1)-C(2)#3	1.554(6)	C(70b)-O(70)	1.450(4)
N(1)-C(9)	1.361(7)	C(70b)-C(71b)	1.528(5)
N(1)-C(5)	1.417(7)	C(71b)-O(71)	1.452(4)
C(2)-C(7)	1.358(8)	O(70)-C(70a)#4	1.450(4)
C(2)-C(3)	1.395(8)	O(70)-C(70b)#4	1.450(4)
N(2)-C(10)	1.326(7)	O(71)-C(71a)#4	1.449(4)
N(2)-C(9)	1.368(7)	O(71)-C(71b)#4	1.452(4)
C(3)-C(4)	1.370(8)		
N(3)-C(9)	1.318(8)	C(2)#1-C(1)-C(2)	103.0(4)
N(3)-C(11)	1.339(8)	C(2)#1-C(1)-C(2)#2	112.82(19)
C(4)-C(5)	1.390(8)	C(2)-C(1)-C(2)#2	112.82(19)
N(4)-C(11)	1.330(8)	C(2)#1-C(1)-C(2)#3	112.82(19)
N(4)-C(10)	1.362(8)	C(2)-C(1)-C(2)#3	112.8(2)
C(5)-C(6)	1.375(8)	C(2)#2-C(1)-C(2)#3	103.0(4)
N(5)-C(11)	1.352(8)	C(9)-N(1)-C(5)	127.4(4)
N(5)-C(16)	1.454(10)	C(7)-C(2)-C(3)	116.1(5)
C(6)-C(7)	1.397(9)	C(7)-C(2)-C(1)	124.5(5)
N(6)-C(10)	1.356(8)	C(3)-C(2)-C(1)	119.4(4)
N(6)-C(12)	1.469(8)	C(10)-N(2)-C(9)	113.1(5)
C(12)-C(13)	1.485(11)	C(4)-C(3)-C(2)	123.1(5)
C(13)-C(14)	1.443(15)	C(9)-N(3)-C(11)	114.1(5)
C(14)-C(15)	1.577(18)	C(3)-C(4)-C(5)	119.3(5)
C(16)-C(17a)	1.46(2)	C(11)-N(4)-C(10)	112.5(5)
C(16)-C(17)	1.58(2)	C(6)-C(5)-C(4)	119.0(5)
C(17a)-C(18)	1.44(3)	C(6)-C(5)-N(1)	124.0(5)
C(17)-C(18)	1.47(3)	C(4)-C(5)-N(1)	116.9(5)
C(18)-C(19)	1.5617	C(11)-N(5)-C(16)	125.3(6)
O(50a)-C(50a)	1.378(5)	C(5)-C(6)-C(7)	119.7(5)
O(50a)-C(53a)	1.379(5)	C(10)-N(6)-C(12)	124.4(5)
C(50a)-C(51a)	1.497(5)	C(2)-C(7)-C(6)	122.7(5)
C(51a)-O(51a)	1.377(5)	N(3)-C(9)-N(1)	120.8(5)
O(51a)-C(52a)	1.379(5)	N(3)-C(9)-N(2)	126.0(5)
C(52a)-C(53a)	1.501(5)	N(1)-C(9)-N(2)	113.1(4)
O(50b)-C(53b)	1.379(5)	N(2)-C(10)-N(6)	117.6(5)
O(50b)-C(50b)	1.380(5)	N(2)-C(10)-N(4)	126.9(5)
C(50b)-C(51b)	1.502(5)	N(6)-C(10)-N(4)	115.4(5)
C(51b)-O(51b)	1.383(5)	N(4)-C(11)-N(3)	127.2(5)
O(51b)-C(52b)	1.380(5)	N(4)-C(11)-N(5)	115.5(5)
C(52b)-C(53b)	1.501(5)	N(3)-C(11)-N(5)	117.3(6)
O(60a)-C(63a)	1.375(5)	N(6)-C(12)-C(13)	112.6(7)
O(60a)-C(60a)	1.375(5)	C(14)-C(13)-C(12)	116.6(9)
C(60a)-C(61a)	1.491(5)	C(13)-C(14)-C(15)	109.8(1)
C(61a)-O(61a)	1.373(5)	N(5)-C(16)-C(17A)	108.70(12)
O(61a)-C(62a)	1.379(5)	N(5)-C(16)-C(17)	112.1(9)
C(62a)-C(63a)	1.498(5)	C(17A)-C(16)-C(17)	57.20(16)
O(60b)-C(63b)	1.383(5)	C(18)-C(17A)-C(16)	117.40(19)
O(60b)-C(60b)	1.386(5)	C(18)-C(17)-C(16)	108.70(11)
C(60b)-C(61b)	1.499(5)	C(17A)-C(18)-C(17)	60.20(15)
C(61b)-O(61b)	1.385(5)	C(17A)-C(18)-C(19)	147.90(12)
O(61b)-C(62b)	1.377(5)	C(17)-C(18)-C(19)	109.7(8)
C(62b)-C(63b)	1.502(5)		

Symmetry transformations used to generate equivalent atoms:

#1 –x,-y+2,z #2 y-1,-x+1,-z
#3 –y+1,x+1,-z #4 –x+2,-y+1,z

Table 6. Torsion angles [°] for C109 H180 N24 O20.

C(2)#1-C(1)-C(2)-C(7)	119.0(6)	C(9)-N(2)-C(10)-N(4)	-0.1(8)
C(2)#2-C(1)-C(2)-C(7)	-2.9(5)	C(12)-N(6)-C(10)-N(2)	7.0(1)
C(2)#3-C(1)-C(2)-C(7)	-119.1(6)	C(12)-N(6)-C(10)-N(4)	-168.6(6)
C(2)#1-C(1)-C(2)-C(3)	-61.9(4)	C(11)-N(4)-C(10)-N(2)	4.1(9)
C(2)#2-C(1)-C(2)-C(3)	176.2(5)	C(11)-N(4)-C(10)-N(6)	179.1(6)
C(2)#3-C(1)-C(2)-C(3)	60.0(3)	C(10)-N(4)-C(11)-N(3)	-5.4(9)
C(7)-C(2)-C(3)-C(4)	-1.5(8)	C(10)-N(4)-C(11)-N(5)	173.9(6)
C(1)-C(2)-C(3)-C(4)	179.2(4)	C(9)-N(3)-C(11)-N(4)	2.4(9)
C(2)-C(3)-C(4)-C(5)	0.2(8)	C(9)-N(3)-C(11)-N(5)	-176.9(6)
C(3)-C(4)-C(5)-C(6)	-0.3(8)	C(16)-N(5)-C(11)-N(4)	-177.1(7)
C(3)-C(4)-C(5)-N(1)	177.4(5)	C(16)-N(5)-C(11)-N(3)	2.30(11)
C(9)-N(1)-C(5)-C(6)	-24.3(8)	C(10)-N(6)-C(12)-C(13)	122.7(8)
C(9)-N(1)-C(5)-C(4)	158.1(5)	N(6)-C(12)-C(13)-C(14)	179.1(9)
C(4)-C(5)-C(6)-C(7)	1.7(8)	C(12)-C(13)-C(14)-C(15)	68.30(13)
N(1)-C(5)-C(6)-C(7)	-175.8(5)	C(11)-N(5)-C(16)-C(17A)	87.90(16)
C(3)-C(2)-C(7)-C(6)	3.0(9)	C(11)-N(5)-C(16)-C(17)	149.30(11)
C(1)-C(2)-C(7)-C(6)	-177.8(5)	N(5)-C(16)-C(17A)-C(18)	72(2)
C(5)-C(6)-C(7)-C(2)	-3.2(9)	C(17)-C(16)-C(17A)-C(18)	–33.20(19)
C(11)-N(3)-C(9)-N(1)	-177.7(5)	N(5)-C(16)-C(17)-C(18)	-68.60(14)
C(11)-N(3)-C(9)-N(2)	2.6(9)	C(17A)-C(16)-C(17)-C(18)	30.00(15)
C(5)-N(1)-C(9)-N(3)	-8.7(9)	C(16)-C(17A)-C(18)-C(17)	34.60(18)
C(5)-N(1)-C(9)-N(2)	171.0(5)	C(16)-C(17A)-C(18)-C(19)	114.10(17)
C(10)-N(2)-C(9)-N(3)	-3.6(8)	C(16)-C(17)-C(18)-C(17A)	–29.50(15)
C(10)-N(2)-C(9)-N(1)	176.7(5)	C(16)-C(17)-C(18)-C(19)	–175.9(7)
C(9)-N(2)-C(10)-N(6)	-175.0(6)		

Symmetry transformations used to generate equivalent atoms:

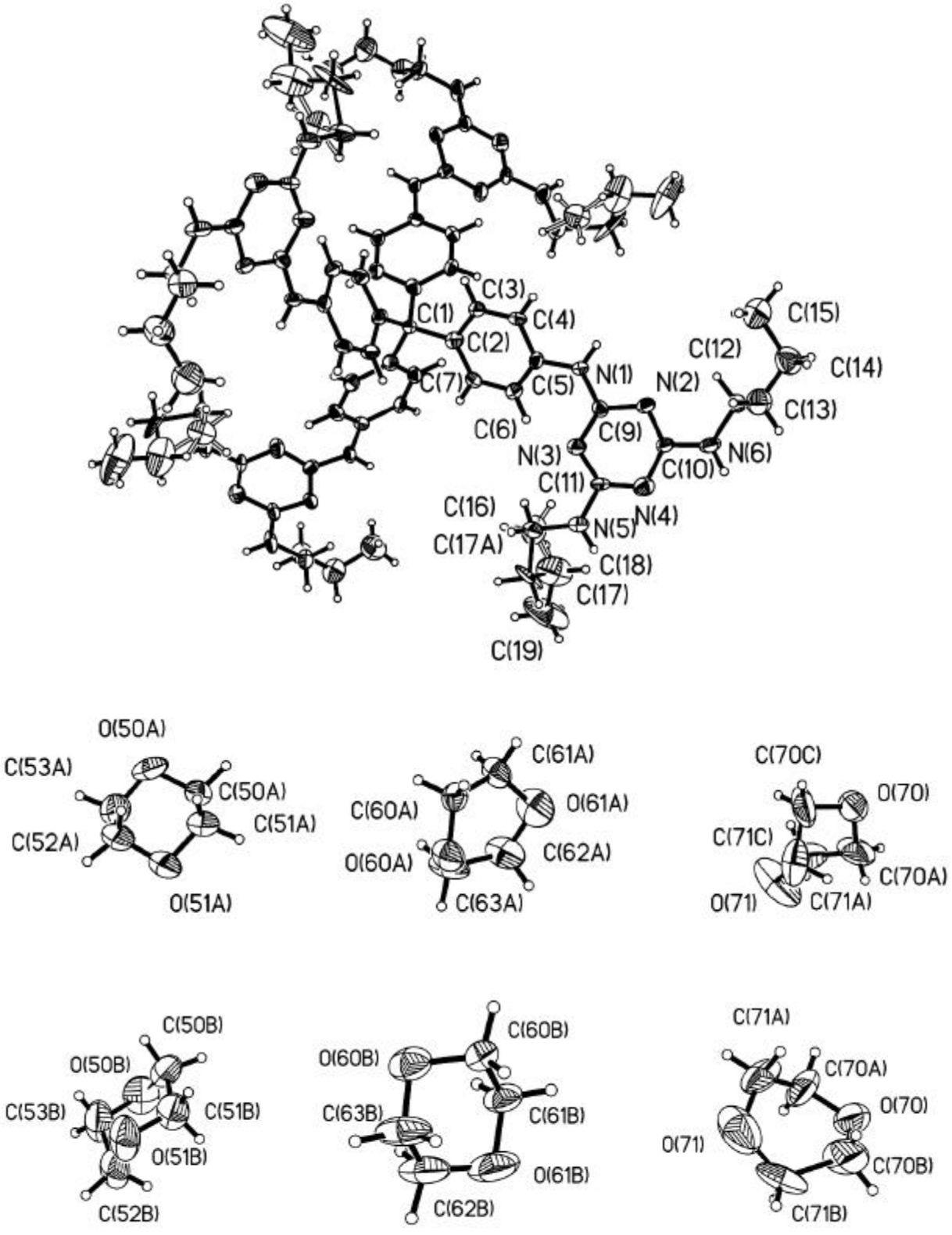
#1 –x,-y+2,z #2 y-1,-x+1,-z
#3 –y+1,x+1,-z #4 –x+2,-y+1,z

Table 7. Bond lengths [Å] and angles [°] related to the hydrogen bonding for C109 H180 N24 O20.

D-H	..A	d(D-H)	d(H..A)	d(D..A)	<DHA
N(1)-H(1A)	N(2)#5	0.87	2.27	3.131(6)	170
N(5)-H(5A)	N(4)#6	0.87	2.19	3.042(8)	164.5
N(6)-H(6A)	O(50B)#7	0.87	2.11	2.89(2)	148.1
N(6)-H(6A)	O(50A)#7	0.87	2.2	3.043(13)	161.9

Symmetry transformations used to generate equivalent atoms:

#1 –x,-y+2,z #2 y-1,-x+1,-z #3 –y+1,x+1,-z
#4 –x+2,-y+1,z #5 –x+1,-y+2,z #6 –x+1,-y+1,z
#7 –y+3/2,x-1/2,-z+1/2



ORTEP view of the C27.25 H45 N6 O5 compound with the numbering scheme adopted. Ellipsoids drawn at 30% probality level Hydrogens represented by sphere of arbitrary size.

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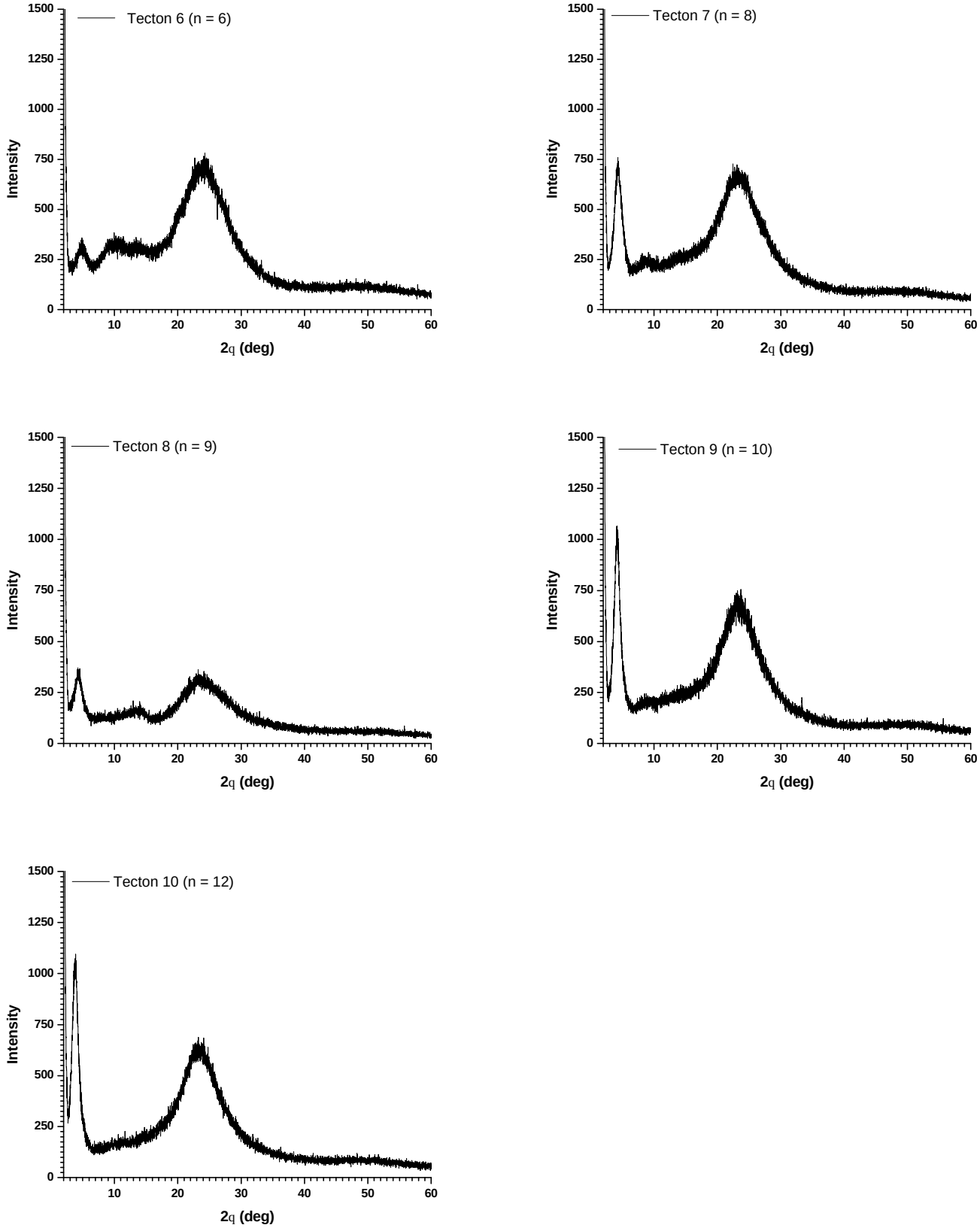

Figure **12**. X-ray diffraction patterns for tectons **6** – **10** in the range 2 – 60 degrees in 2θ.

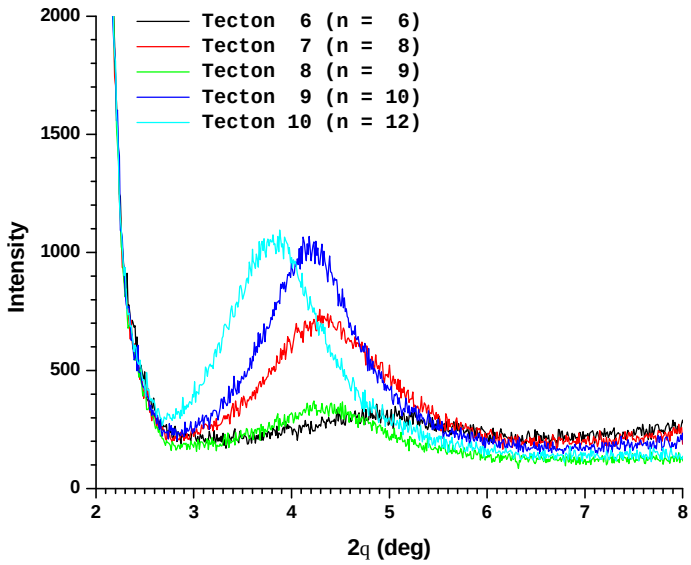

Figure **13**. X-ray diffraction patterns for tectons **6** – **10** plotted in the range 2 – 8 degrees in 2θ.

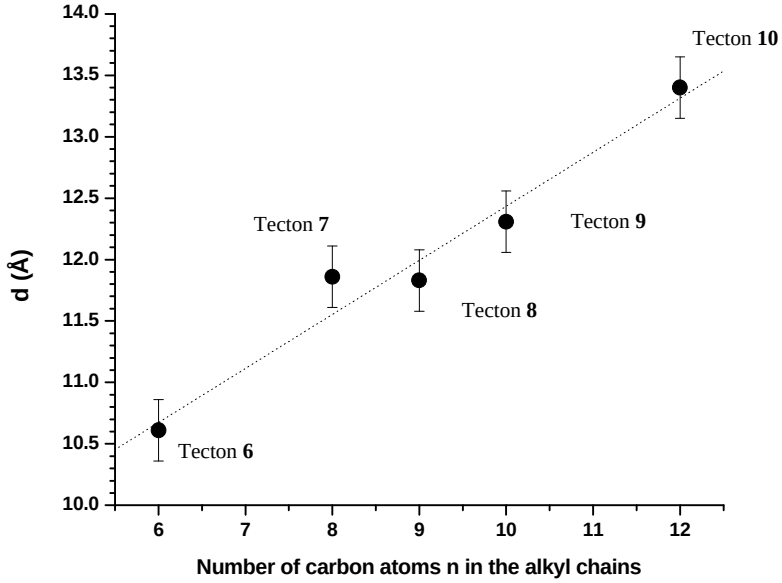

Figure **14**. Plot of the reticular distance against the alkyl chain lenght measured from the first diffraction line at low angle for tectons **6** – **10**.